

Open Data Lab Annual Report - 2018

The Open Data Lab Collaboration

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The Team



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Phil Bourne "At vero eos et accusamus et iusto odio dignissimos ducimus qui blanditiis praesentium voluptatum deleniti atque corrupti quos dolores et quas molestias excuri sint occaecati cupiditate non provident,At vero eos et accusamus et dent,"



Tim Clark "Tim Clark, Ph.D., is a biomedical informatician and computer scientist with 28 years experience in academic, government and industry. He is an expert in biomedical knowledge representation, data fusion and open science applications. He is an Associate Professor appointed in the UVA School of Medicine & the Data Science Institute."



Max Levinson "Max Levinson is a Software Engineer and Cloud Developer within Public Health Services. When not building out REST apis for the NIH Data Commons Project, he can be found hacking on the Open Data Lab Project. Max is passionate about microservices development, knowledge graphs, and anything python."



Daniel Mietchen "At vero eos et accusamus et iusto odio dignissimos ducimus qui blanditiis praesentium voluptatum deleniti atque corrupti quos dolores et quas molestias excuri sint occaecati cupiditate non provident,At vero eos et accusamus et dent,"



Lane Rasberry "At vero eos et accusamus et iusto odio dignissimos ducimus qui blanditiis praesentium voluptatum deleniti atque corrupti quos dolores et quas molestias excuri sint occaecati cupiditate non provident,At vero eos et accusamus et dent,"

Letter from the editor

hello world

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Chapter 1

Overview

1.1 What is the Open Data Lab?

OPEN

We encourage all users to be as open as possible with every aspect of their work. That may be in opening up their data sets, publication, source code, or ...

DATA

We take an expansive definition of data. Everything from traditional data, to code, to workflows, to published material, and so on is considered data to us. We provide a place for all things digital data.

LAB

We provide a place where the power of contemporary computing can be brought to bear against data resources. Given the scale of data today this means colocating the data and computational resources.

Open Data Lab

The Open Data Lab is a resource to provide state of the art computing and data infrastructure to researchers, students, and sharers. It is guided by the principles of science and openness.

1.2 User Archetypes

There are many potential use cases for the Open Data Lab. In this section we describe the three cases that have been tested so far. They are: the Collaborator, someone who is working on a research project; the Student, someone who is using the Open Data Lab to learn about data science; and the Sharer, a person with data who wants to open it up to a broader audience.

The Collaborator

This archetypal person uses the Open Data Lab to conduct research. They access data and computational resources that are colocated. This colocation facilitates lower latency and increased performance. A wide range of services can be provided globally by AWS and locally through UVA HPC resources. Sample workflow:

1. Request a user account on the Open Data Lab
2. Once per collaboration:
 - (a) Load data
 - (b) Provision computational resources
3. Conduct research operations
4. Register resulting products in Dataverse

The Student

This archetype uses the Open Data Lab to facilitate learning. An example would be someone who participates in a workshop where an ODL notebook instance powered by AWS SageMaker provides the working environment. Sample workflow:

1. Request a user account on the Open Data Lab
2. Logon to AWS console to launch Jupyter
3. Use Jupyter during the workshop

The Sharer

This archetype is a user who owns data and wants to make it available. There are many mechanisms for sharing the data ranging from RESTful API of S3, to a SPARQL endpoint. Sample workflow:

1. Request a user account on the Open Data Lab
2. Load data into an S3 bucket
3. Configure one of the following
 - (a) SPARQL endpoint
 - (b) API Gateway to access S3
 - (c) S3 permissions for a SageMaker notebook
 - (d) ...

1.3 User Summary

group	projectID	# members	type
Bourne-Mura	bamc	4	MSDS Capstone
CBW	cbwc	4	MSDS Capstone
Wiki	wiki	9	MSDS Capstone
Mental Health	miip	6	SYS Capstone
Women Terror Recruitment	watr	2	Presidential Fellow
Healthy Markets	hmtt	5	DSI Research
Independent Study	pmis	1	DSI Research
Linked Open Data	nept	2	External Data
Spark	sprk	17	Education
GitHub	gith	9	Education
ORCI	orci	2	ODL Development
ML under	mlunder	7	Club
ML grad	mlgrad	3	Club
Rivanna	—	11	Local
Ivy	—	6	Local
ODL-education	—	26	Education Users
ODL-users	—	68	Unique Users

1.4 A phased approach

The first three phases of the Open Data Lab have been outlined. Phase 0 focused on pre investigation and decided on what technology to test in Phase 1, the closed beta. Phase 2 is an open Beta and will serve the community of Charlottesville and other associated research and educational efforts.

Phase	type	start	end
0	alpha	FEB 2018	JUN 2018
1	closed beta	JUL 2018	MAY 2019
2	open beta	TBD	-

Short Term Goals

1. Explore technology to solve open Open Data Lab questions
2. Serve Data Science Institute users
3. Understand user archetypes

Long Term Goals

Change the way science is done.

1.5 What's next for the Open Data Lab?

The year 2019 will be a big year for the Open Data Lab. The gathering of information and skill from the closed beta has gone well. While continuing the closed beta through the spring semester 2019 the Open Data Lab will be seeking to add staff to prepare for the open beta launch.

Chapter 2

Key Developments

This year saw great progress for the Open Data Lab. Early on there were weekly meetings to define goals and objectives. Those meetings lead to implementation of several areas and this chapter presents the key developments during 2018.

2.1 Phase 1 - Closed β

The first decision made for the Open Data Lab was to implement a staged approach. Section 1.4 summarizes the whole scope. This section discusses the state of the closed beta (Phase I). The user base for this phase is predominantly the Data Science Institute. There were 42 participants ranging from students, to faculty, to staff. There were also 26 workshop attendees ranging from a diverse selection of UVA researchers to community members. The primary goal of this phase is to test different technology solutions to anticipated needs (see section 2.3. Those range from data storage to computation to discovery to pedagogy, and so on. Of particular note was the wild success of implementing Project Jupyter. The tools developed by this project served many roles and were excellent (details in section 2.3.1. This phase will run until several criteria are met. The first is the establishment of a new funding model that will cover the scope of the open beta test. The second is the acquisition of new staff. Currently the Open Data Lab has a bus factor of one and that is not acceptable for phase 2. There are other criteria to be developed the chief of which is to scope the open beta.

2.2 Establishment of User base

This year saw the birth of the Open Data Lab and growth to include 68 users. Those users take various form from capstone research programs at the graduate and undergraduate level to full fledged dissertation research. Some of the users involved are dealing with datasets that now reside within the Open Data Lab. Currently those datasets are under tight restriction as we explore proper security protocols. There is also a contingent of undergrad and graduate students that are part of data science clubs at UVA who gain access to resources through the Open Data Lab.

It is important to understand that the technology behind the system is not the driver of the system. The needs of the user are. Right now the closed beta format allows us to interview new users and tailor a program to them. Sometimes we get the resource wrong and adjustments have to be made. Regarding data storage the use of S3 storage from Amazon Web Services has served a broad selection of users well. Recent developments in AWS object storage technology enable users to use it as if it were block storage. As a result S3 has proved an effective solution both for large scale data storage as well as database query repositories. Providing computational resources has been guided by the user base as well. As the base grew it became clear that the notebook technology developed by Project Jupyter was highly effective and actually resulted in more people volunteering for the closed beta test. The use of that technology helped bring users into the system.

2.3 Technology Exploration

Many different technologies were tested in 2018. Many options using Amazon Web Services were explored and almost to a point those services were excellent. Local UVA resources were also used and in particular the UVA HPC portal developed out of the VP-IT's office is phenomenal. Collaboration is also underway with the UVA library regarding the discovery component of the Open Data Lab and the implementation of Harvard's Dataverse, known locally at UVA as Libra. For version control and sharing purposes GitHub was evaluated.

2.3.1 Amazon Web Services

S3

EC2

SageMaker (Jupyter)

IAM

API Gateway

Architecture Diagrams

lambda

13 TB Data Transfer

Usage Report

Support Plan

<https://aws.amazon.com/premiumsupport/compare-plans/>

2.3.2 Local UVA - Rivanna and Ivy

The local computational resources at UVA are facilitated through the office of Vice President for IT. That group is dedicated and hard working and provides great resources to the local UVA community. We have established a working relationship with them and discuss technical problems and solutions. Independently we arrived at the utility of Project Jupyter. These solutions are for UVA personnel and their collaborators and as such will not scale to later phases of the Open Data Lab project. However for the closed and open beta it is a great resource. Furthermore their technical expertise will be invaluable to the Open Data Lab regardless of phase.

2.3.3 GitHub

GitHub is the most broadly adopted cloud platform for version control. Therefore we evaluated it first. The utility for managing repositories is fully mature. The collaborative features focused around the fork and pull request paradigm are excellent. GitHub also has project level capability with issue tracking and team/permission functionality for managing permissions and

progress. We have been extremely pleased with the capabilities of GitHub. The only motivation to try other solutions is for the sake of due diligence.

Concerning the acquisition by Microsoft: Many have raised the issue that GitHub may not be the appropriate solution now that Microsoft has acquired GitHub. However the recent track record of Microsoft is to not meddle with projects like GitHub but rather to protect them. Additionally most users use other Microsoft products. What's more the Open Data Lab also relies heavily on Amazon.

2.4 Upcoming Technical Exploration

The following sections describe exploratory work that is on the schedule. There is more to be done beyond this list but not scheduled.

2.4.1 Dataverse

A framework has been outlined to use Dataverse as the discovery mechanism for the Open Data Lab. In this system a metadata entry will be made in the Dataverse containing all of the usual materials. However the final piece with the datafiles will contain pointers to the data and projects within the Open Data Lab. Dataverse is not configured for colocating computation resources with the data resources. The pilot of this test will be with the Libra project from the UVA Library. Currently that system is undergoing an upgrade and once there is a stable release exploration will commence.

2.4.2 Spark

The first scale data solution the Open Data Lab will explore is Spark. Preliminary work so far as been the development of a introductory workshop on the technology (available on the Open Data Lab github repository). A second pedagogical series will be presented early in 2019 and will lead to testing different technical solutions.

2.4.3 SPARQL Endpoint

The numismatic dataset will be accessible through a SPARQL endpoint. This exploration is in the early stage and has not matured to the point of

evaluation. The next annual report will have a full breakdown of the best way to treat this form of data and delivery.

Chapter 3

Datasets

3.1 Healthy Markets

3.2 Numismatic

Chapter 4

Research

4.1 Bourne/Mura Capstone

4.2 DSI Wiki

Chapter 5

Education

A key component of openness is making resources usable. This idea falls in line with the idea that openness and accessibility are part of the same mission. As a result the educational component of the Open Data Lab is vital to the success of the project. There are two main thrusts in this endeavor. The first, which was piloted in 2018, is the production of educational materials and methods. The second part is the development of communication paradigms. This year two workshops were produced and delivered as part of the closed beta test. The first focused on the scale data protocol spark and the second the version control tool GitHub.

5.1 Spark Workshop

This workshop was designed as an introduction to spark. The goals were:

- Teach how to get started
- Build comfort
- Teach how to get answers to further questions

The topics covered included linking to a spark context, reading in data via dataframes, manipulating the data, and making a fundamental calculation. To power the workshop the attendees were given credentials on a Amazon SageMaker notebook. One of the features of this approach is that the whole workshop has access to the same environment. Everyone sees the same implementation of the software and hardware. There is no cumbersome overhead

in getting set up. The requirements are a web browser and access to the internet. Furthermore the single notebook environment leads to a very useful pedagogical capability. When a student encounters an error in their code the instructor can load their notebook on the main display in the room. In real time and in full view of everyone the instructor can debug and teach the whole class. This is a vast improvement over the current popular method of hovering over a single learners station. It enables every person in the room to see what is going on and maintain their level of engagement. This experience was very positive for the learners and the feedback to this approach was superlative. Previous versions of spark training was done with Databricks resources and there were several drawbacks precipitating the switch to Amazon.

- The environment is not shared between the workshop participants and the instructor
- Every learner independently established their own cluster and there is substantial lag
- Materials must be imported in Databricks format (.dbc) instead of more universal jupyter notebook format (.ipynb).

Resources:

- Databricks based workshop can be found at: <https://github.com/alonzi/spark>
- Amazon Sagemaker based workshop can be found at: <https://github.com/alonzi/spark-intro>
- Next generation materials will be incorporated into the Open Data Lab repository at: <https://github.com/UVA-DSI/Open-Data-Lab/tree/master/education>

The cost to operate and instructional environment is \$0.0464 per hour. For this workshop we ran the environment for one week at a cost of approximately \$10.

5.2 GitHub Workshop

The Open Data Lab was invited to present GitHub to the Archaeology Department of the Thomas Jefferson Foundation (aka Monticello). We developed a workshop to explain the fundamentals of version control and present

a work-flow for beginning users. The different user archetypes were also discussed. One of the major burdens to version control use is that it comes from the computer superuser community. Most of the software is developed using a terminal based interface (CLI). However in today's research world many one computer superusers interact with code and other materials that benefit from a version control workflow. The major benefit from GitHub is the browser based interface. This implementation shifts substantial pieces of cognitive load off the user. This shift enables the user to focus on developing their work rather than on the bookkeeping of version controlling their work. At the same time it makes it easy for the developers to take advantage of the version control benefits. There is substantial room to further develop materials for different user archetypes. This workshop focused on a research group. We will strive to identify other archetypes and develop materials to suit those needs. This workshop was taught straight from the GitHub repository itself. That was a natural fit given the subject matter. But it also demonstrated several very useful pieces of GitHub as a teaching medium, which will be discussed in 5.3.

Resources: <https://github.com/UVA-DSI/Open-Data-Lab/tree/master/education/GitHub>

5.3 Using GitHub as a Teaching Medium

Both of the workshops taught under the Open Data Lab project used GitHub as the repository for materials. This has several benefits.

- GitHub provides a URL and free hosting for resources
- Subsequent changes to the materials are stored under version control thus allowing the actual materials presented to be recovered
- Any learner who wants to suggest improvements to materials can implement a pull request

The decision to put the materials in GitHub was one of necessity since the Open Data Lab GitHub page serves as the repository for all Open Data Lab resources. GitHub by default provides a URL for every item stored in the repository and presents the README file of a repo. This presentation is automatically rendered from markdown. Wikipedia has demonstrated the success of using markdown for content presentation but to enumerate some

key features here. The document is organized, hyperlinkable, figures are easily embeded, and it seamlessly renders text alongside code and mathematical formulae.

5.4 Plans for 2019

The Open Data Lab is scheduled to teach several workshops in 2019:

- A five part series on Spark for the DSI MSDS cohort
- A three part series for the UVA Library on Python and Machine Learning
- Likely another three part series for the UVA Library in Fall 2019
potential collab with COS?

Chapter 6

Vital Metrics

6.1 AWS usage

6.2 FTE analysis

6.3 Budget

6.3.1 Funding

funded by the Data Science Institute healthy markets project funded off-budget for ODL